Numerical Continuation of Bifurcations —- An Introduction, Part I

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Outline

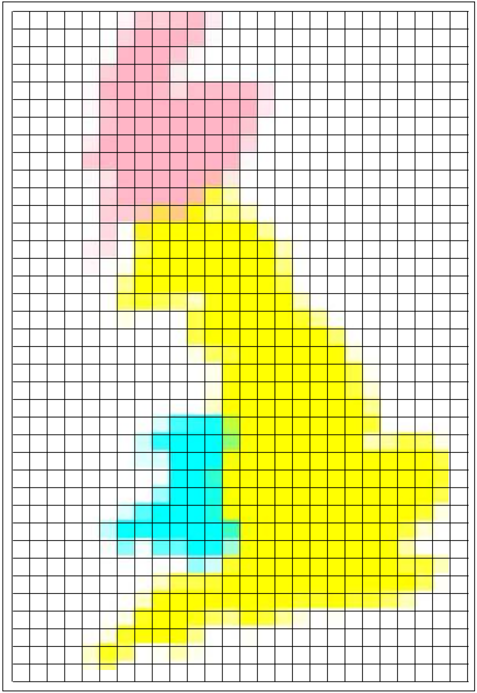
- Continuation — motivation
- pseudo-arclength continuation
- Boundary value problems
- Periodic orbits
- Detection of bifurcations (later)
- Continuation of bifurcations (later)
- Further reading/software

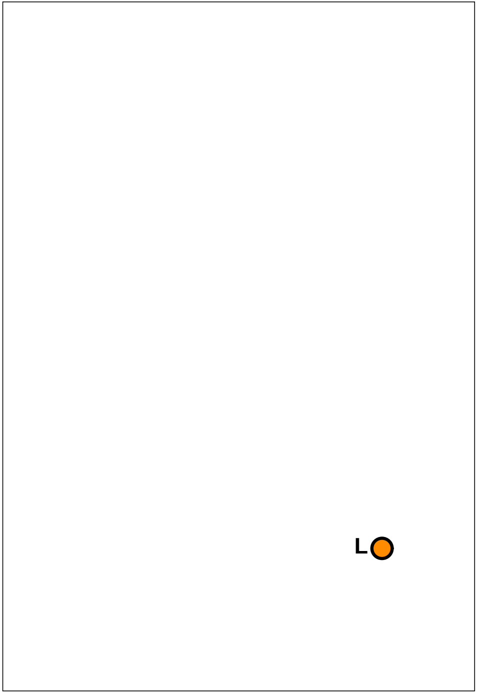
Motivation for Using Continuation Techiques

(see Krauskopf/Lenstra: *Fundamental Issues of Nonlinear Laser Dynamics*, 2000)

- Problem: discover UK mainland, classify into England, Wales, Schottland
- Alternative A: ‘Simulation’, test on a fine grid of points
- Alternative B: ‘Continuation’,
  - start in point you know (L),
  - go ahead, always checking were you are
  - detect borders
  - go along borders
  - detect cross points
  - branch off at cross points

$\Longrightarrow$flip through animation on next slide

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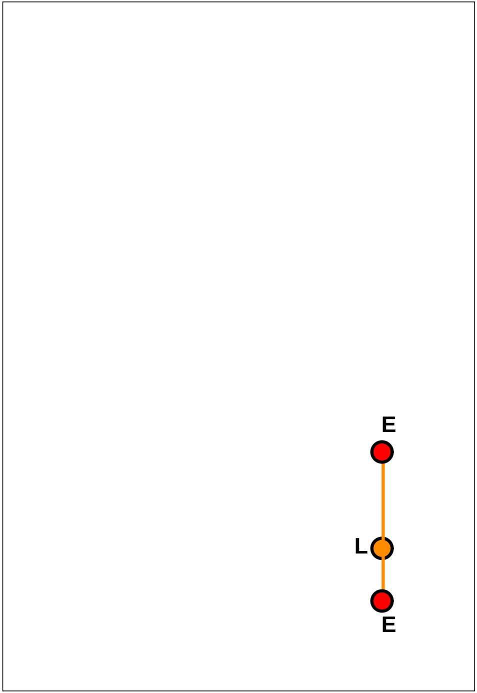
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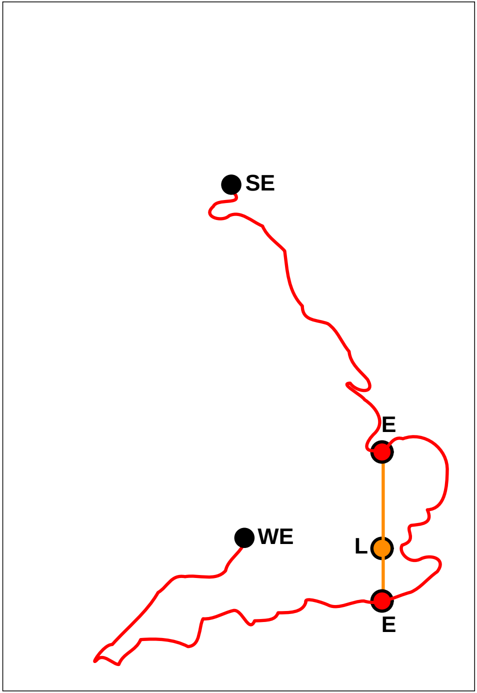
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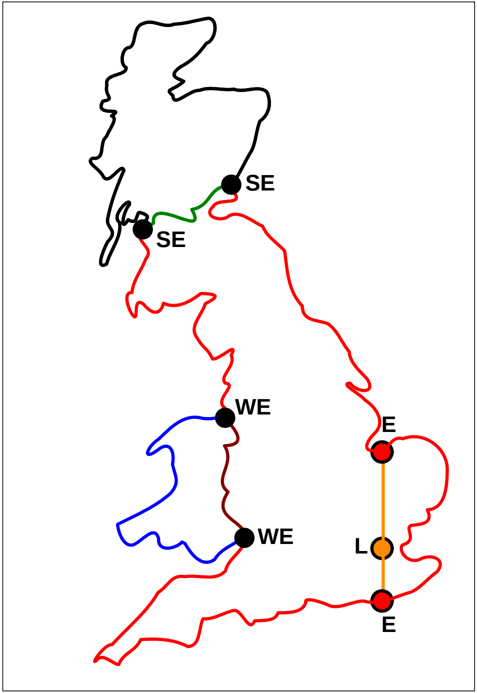
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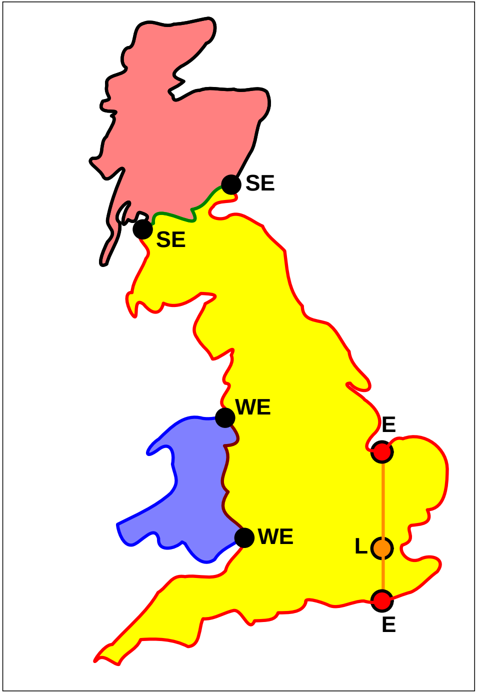
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Newton iteration

- Solve **nonlinear** system of equations

$$f(x) = 0, \quad f : \mathbb{R}^n \mapsto \mathbb{R}^n, \quad x \in \mathbb{R}^n, \quad p \in \mathbb{R}$$

- Initial guess $x_0 \in \mathbb{R}^n \Longrightarrow$iteration

$$x_{k+1} \quad = \quad x_k - [\partial f(x_k)]^{-1} f(x_k)$$

- Assumption: Solution x_* exists, is regular
$\Longrightarrow \det \partial f(x_*) \neq 0$
- Pro: good convergence
- Con: $x_0 \approx x_*$ required

Parameter Continuation

- Find $x \in \mathbb{R}^n$ s.t.

$$f(x,p) = 0, \quad f : \mathbb{R}^n \times \mathbb{R} \mapsto \mathbb{R}^n, \quad p \in \mathbb{R}$$

- Assumption:
  solution for p_0 known: $f(x_0, p_0) = 0$, $\partial_1 f(x_0, p_0)$ regular
- Implicit Function Theorem $\Longrightarrow$
  solution curve $x(p)$ for $f(x(p), p) = 0$
- iterate:
  1. choose $p_{k+1} \approx p_k \Longrightarrow$
  2. old solution x_k initial guess for $f(x, p_{k+1}) = 0$
  3. solve $f(x, p_{k+1}) = 0$ with Newton iteration $\Longrightarrow x_{k+1}$
- points (x_k, p_k) on solution curve $x(p)$
- fails if $\partial_1 f(x_0, p_0)$ not regular

Pseudo-arclength continuation

- Find $y \in \mathbb{R}^{n+1}$ s.t.

$$f(y) = 0, \quad f : \mathbb{R}^{n+1} \mapsto \mathbb{R}^n$$

- Assumption: $y_0, z_0 \in \mathbb{R}^{n+1}$ s.t. $f(y_0) = 0$, $\dim \operatorname{rg} \partial f(y_0) = n, \quad \partial f(y_0) z_0 = 0$.
- Implicit function theorem $\Longrightarrow$solution curve $y(s)$ ($s \in (-\delta, \delta)$), s.t. $f(y(s)) = 0, \quad y(0) = y_0, \quad y'(0) = z_0$.

- **Iteration**
  1. predictor step $y_{k+1}^P = y_k + hz_k$
  2. corrector step $\Longrightarrow$
     Newton iteration for y_{k+1}

$$\begin{aligned} 0 &= f(y_{k+1}) \\ 0 &= z_k^T \cdot (y_{k+1} - y_{k+1}^P) \end{aligned}$$

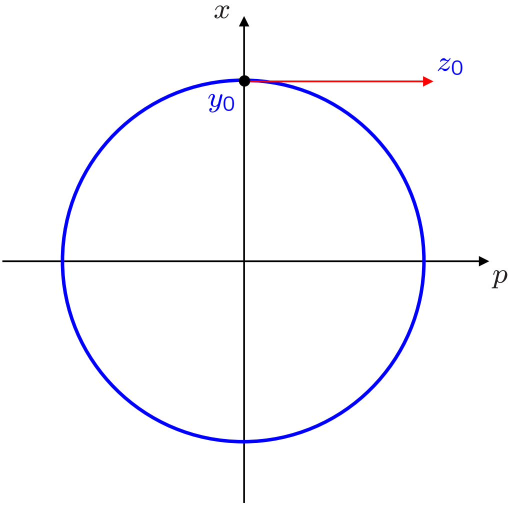
     with initial guess $y_{k+1} = y_{k+1}^P$
  3. new tangent

$$\begin{aligned} 0 &= \partial f(y_{k+1}) z_{k+1} \\ 1 &= z_k^T \cdot z_{k+1} \end{aligned}$$

- if y_k is on solution curve $\Longrightarrow$Jacobian $\in \mathbb{R}^{(n+1)\times(n+1)}$ regular

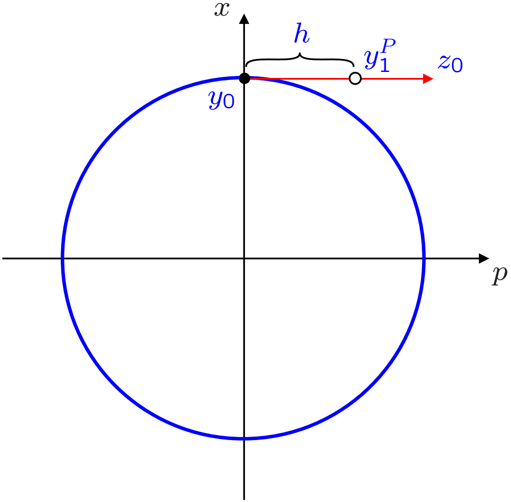
$$\begin{bmatrix} \partial f(y_k) \\ z_k^T \end{bmatrix}$$

Geometric illustration



$$
\begin{aligned}
y &= (x, p) \\
0 &= f(y) \\
&= x^2 + p^2 - 1
\end{aligned}
$$

Geometric illustration



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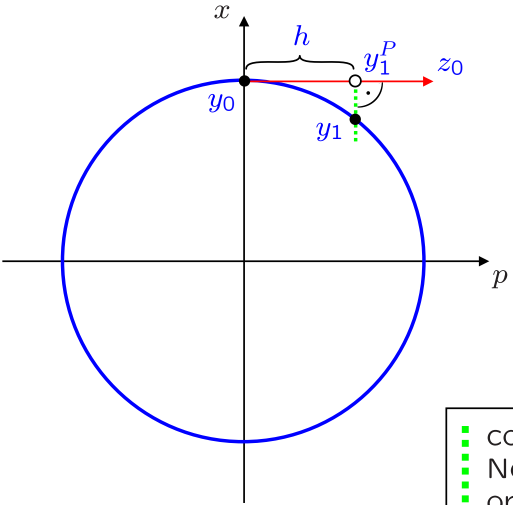
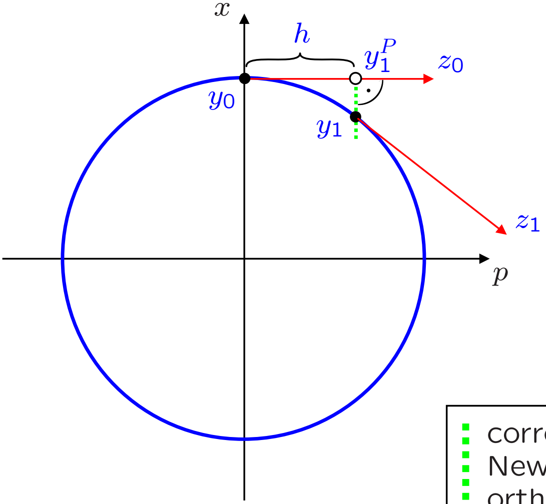


$$y = (x, p)$$
$$0 = f(y)$$
$$= x^2 + p^2 - 1$$

stepsize $h \ll 1$

- corrector step
- Newton iteration
- orthogonal to tangent

Geometric illustration



$$y = (x, p)$$
$$0 = f(y) = x^2 + p^2 - 1$$

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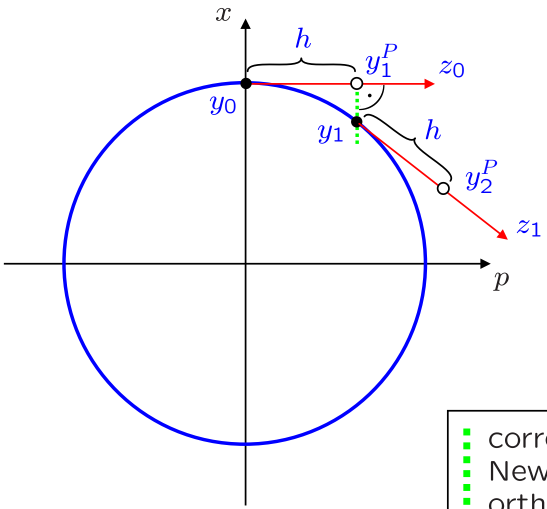
Geometric illustration



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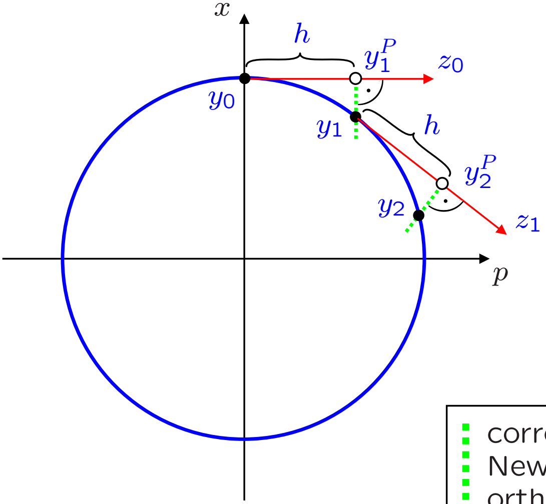

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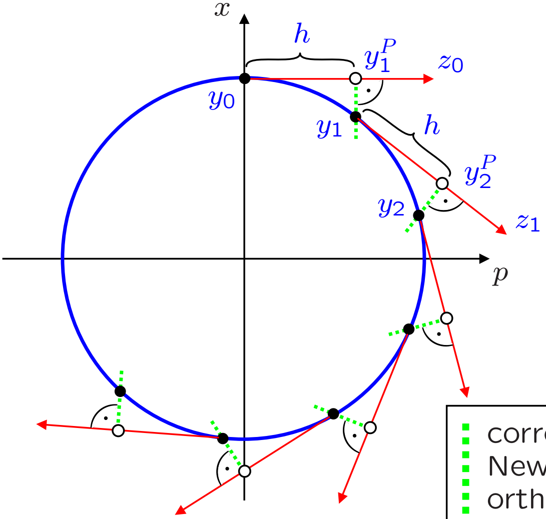

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Boundary Value Problems (BVP)

- solution $u(\cdot) \in \mathbb{R}^{n_{\text{dim}}}$ of dimension n_{dim}
- parameter $p \in \mathbb{R}^{n_{\text{cp}}}$ of dimension n_{cp}
- u solves differential equation (ODE) on interval $[0, 1]$

$$\dot{u}(t) = f(u(t), p)$$

- with n_{bc} boundary conditions

$$g(u(0), u(1), p) = 0, \qquad g : \mathbb{R}^{2n_{\text{dim}}+n_{\text{cp}}} \mapsto \mathbb{R}^{n_{\text{bc}}}$$

- and n_{int} integral conditions

$$\int_0^1 h(u(t), p)\, dt = 0, \qquad h : \mathbb{R}^{n_{\text{dim}}+n_{\text{cp}}} \mapsto \mathbb{R}^{n_{\text{int}}}$$

- initial value problem generates flow map Φ

$$\dot{u}(t) = f(u(t), p), \qquad u(0) = x$$

$\Longrightarrow u(t) = \Phi(t; x) \qquad (\Phi(0; x) = x)$

- BVP is nonlinear system with $n_{\text{dim}} + n_{\text{cp}}$ variables (x, p) and $n_{\text{bc}} + n_{\text{int}}$ equations

$$0 = g(x, \Phi(1; x), p)$$
$$0 = \int_0^1 h(\Phi(t; x), p)\, dt$$

- pseudo-arclength continuation for $y = (x, p)$ possible if $n_{\text{dim}} + n_{\text{cp}} = n_{\text{bc}} + n_{\text{int}} + 1$

Discretization

- subdivide interval $[0, 1]$ into N subintervals I_k

$$0 = t_0 < t_1 < \ldots t_N = 1$$

- in each subinterval $I_k = [t_{k-1}, t_k]$:
  approximate solution $u(t)$ by polynomial of order m:

$$u(t) \approx q_k(t) \qquad \text{for} \qquad t \in I_k$$

- q_k satisfies ODE at m points in I_k: t_k^j, $j = 1 \ldots m$
  Gauss points (orthogonal collocation)
  $\Longrightarrow$error of order N^{-2m}.
- + continuity conditions, boundary conditions, integral conditions

Equations and Variables

- **Variables:**
  $N \cdot (m+1) \cdot n_{\text{dim}}$ coefficients of polynomials q_k,
  n_{cp} parameters
- **Equations:**
  - ODE: $\dot{q}_k(t_k^j) = f(q_k(t_k^j), p)$ for $j = 1 \dots m$, $k = 1 \dots N$
    $\Longrightarrow N \cdot m \cdot n_{\text{dim}}$ equations
  - Continuity: $q_k(t_k) = q_{k+1}(t_k)$ for $k = 1 \dots N-1$
    $\Longrightarrow (N-1) \cdot n_{\text{dim}}$ equations
  - Boundary conditions: $g(q_1(0), q_N(1), p) = 0$
    $\Longrightarrow n_{\text{bc}}$ equations
  - Integral conditions: $\sum_{k=1}^{N} \int_{I_k} h(q_k(t), p)\, dt = 0$
    $\Longrightarrow n_{\text{int}}$ equations
- $\Longrightarrow N \cdot (m+1) \cdot n_{\text{dim}} + n_{\text{cp}}$ variables,
  $\Longrightarrow N \cdot (m+1) \cdot n_{\text{dim}} - n_{\text{dim}} + n_{\text{bc}} + n_{\text{int}}$ equations

Continuation of Periodic Orbits

- $u(t)$ is periodic orbit of

$$\dot{u}(t) = f(u(t), p)$$

  if it satisfies for some period T the boundary condition

$$u(0) - u(T) = 0$$

- period T is unknown
- Phase invariance $\Longrightarrow u$ is not unique:
  if $u(t)$ is periodic then $u(t + \delta)$ is periodic
- How to set up a regular BVP?

- rescale time:

$$\dot{u}(t) = Tf(u(t), p) \qquad \Longleftarrow \text{ODE}$$
$$0 = u(0) - u(1) \qquad \Longleftarrow \text{boundary c.}$$

- T additional free parameter $\Longrightarrow$ one additional condition to fix phase
- for example: Poincaré section: $u_k(0) = \text{fixed}$ for some $k \leq n_{\text{dim}}$
- computationally optimal for mesh-adaption during continuation

$$0 = \int_0^1 \dot{u}_{\text{old}}(t)^T u(t)\, dt$$

where u_{old} is the previous solution along the branch
This guarantees

$$\int_0^1 \|u_{\text{old}}(t) - u(t)]\|^2\, dt \to \min$$

Continuation of Periodic Orbits

- final form

$$\begin{aligned} \dot{u}(t) &= Tf(u(t), p) && \Longleftarrow \text{ODE} \\ 0 &= u(0) - u(1) && \Longleftarrow \text{boundary c.} \\ 0 &= \int_0^1 \dot{u}_{\text{old}}(t)^T u(t)\, dt && \Longleftarrow \text{integral c.} \end{aligned}$$

- $n_{\text{bc}} = n_{\text{dim}}, n_{\text{int}} = 1$
  $\Longrightarrow$continuation needs $n_{\text{cp}} = 2$ parameters:
  p (one-dimensional) and period T
- continuation variable y consists of $(u(\cdot), p, T)$

Bifurcation detection — equilibria

Special functions (as used by AUTO) for continuation of equilbria

$$0 = f(y) = f(x, p)$$

- Fold (turning point, saddle-node): $z_{k,n+1}/\|z_k\|$
  (last component of tangent vector)
- Hopf (equilibria): imaginary part of complex eigenvalues of $\partial_1 f(x_k, p_k)$
- Branching point:

$$\det \begin{bmatrix} \partial f(y_k) \\ z_k^T \end{bmatrix}$$

Bifurcation detection — periodic orbits

Continuation variable
$y = (u([t_k^j, t_k]), p, T)$ for $k = 1 \ldots N$, $j = 1 \ldots m$
overall dimension $n = N \cdot m \cdot n_{\text{dim}} + n_{\text{cp}}$

- Fold (for general BVP) $z_{k,n-n_{\text{cp}}+1}/\|z_k\|$,
  for periodic orbits $z_{k,n-1}/\|z_k\|$
- Branching points: determinant of *reduced* linearization
- Period doubling, Torus bifurcation: magnitude of Floquet multipliers (excluding one trivial Floquet multiplier 1)
- see Kuznetsov '04: *Elements of Applied Bifurcation Theory* for alternatives

Continuation of Bifurcations — Equilibria

Fully extended systems (see Kuznetsov '04 for alternatives):
Fold:

- variables $x, v \in \mathbb{R}^n$, $p \in \mathbb{R}^2$,
- v nullvector of linearization
- equations:

$$\begin{aligned} 0 &= f(x, p) \\ 0 &= \partial_1 f(x, p) \cdot v \\ 1 &= v^T v \end{aligned}$$

- $\Longrightarrow 2n + 2$ variables, $2n + 1$ equations

Continuation of Bifurcations — Equilibria

Hopf:

- variables x, q_r, $q_i \in \mathbb{R}^n$, $r_\omega \in \mathbb{R}$, $p \in \mathbb{R}^2$
- $q_r + iq_i$ eigenvector for imaginary eigenvalue ir_ω^{-1}
- equations:

$$
\begin{aligned}
0 &= f(x, p) \\
0 &= \begin{bmatrix} r_\omega \partial_1 f(x,p) & I \\ -I & r_\omega \partial_1 f(x,p) \end{bmatrix} \begin{bmatrix} q_r \\ q_i \end{bmatrix} \\
1 &= q_r^T q_r + q_i^T q_i \\
0 &= q_{i,\text{old}}^T (q_r - q_{r,\text{old}}) - q_{r,\text{old}}^T (q_i - q_{i,\text{old}})
\end{aligned}
$$

- $\Longrightarrow 3n + 3$ variables, $3n + 2$ equations
- period of periodic solution branch will be $2\pi r_\omega$

Continuation of Bifurcations — Periodic Orbits

Fold (for other bifurcations see AUTO or Kuznetsov):

- variables: $u(\cdot)$,$v(\cdot) \in \mathbb{R}^n$ on $[0, 1]$, $p \in \mathbb{R}^2$, T, $\beta \in \mathbb{R}$
- v generalized eigenvector of Floquet multiplier 1, T period
- equations:

$$\dot{u} = Tf(u, p) \qquad \Longleftarrow \text{ODE}$$

$$\dot{v} = T\partial_1 f(u, p)v + \beta f(u, p) \qquad \Longleftarrow \text{ODE}$$

$$0 = u(0) - u(1) \qquad \Longleftarrow \text{boundary c.}$$

$$0 = v(0) - v(1) \qquad \Longleftarrow \text{boundary c.}$$

$$0 = \int_0^1 \dot{u}_{\text{old}}(t)^T u(t)\, dt \qquad \Longleftarrow \text{integral c.}$$

$$0 = \int_0^1 \dot{u}_{\text{old}}(t)^T v(t)\, dt \qquad \Longleftarrow \text{integral c.}$$

$$c = \int_0^1 v(t)^T v(t)\, dt + \beta^2 \qquad \Longleftarrow \text{integral c.}$$

Further software

- AUTO
  - current versions: **AUTO97** (fortran), **AUTO2000** (C, python)
  - documentation: manual, lecture notes on http://indy.cs.concordia.ca/auto/
  - help for AUTO2000 (and 97): Bart Oldeman
- software performing similar tasks:
  - **MATCONT** (implemented in Matlab), currently maintained at Gent (Belgium), http://www.matcont.ugent.be
  - **XPPAUT** (simulation package has interface for AUTO) http://www.math.pitt.edu/~bard/xpp/xpp.html
- Delay-differential equations: DDE-BIFTOOL, PDDECONT
- invariant manifolds:
  - invariant tori (**Torcont**)
  - 1D stable/unstable manifolds of periodic orbits (part of **DsTool**)
- see http://www.dynamicalsystems.org/sw/sw/ for more